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ABSTRACT and SLIDES

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CFD Modeling for Mercury Control Technology

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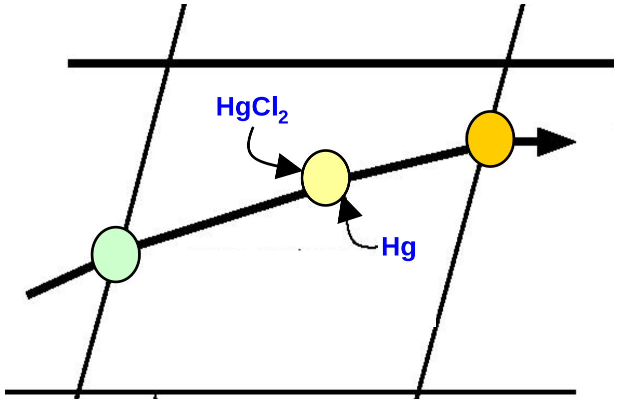
Compliance with the Clean Air Mercury Rule will require implementation of dedicated mercury control solutions at a significant portion of the U.S. coal-fired utility fleet. Activated Carbon Injection (ACI) upstream of a particulate control device (ESP or baghouse) remains one of the most promising near-term mercury control technologies. The DOE/NETL field testing program has advanced the understanding of mercury control by ACI, but a persistent need remains to develop predictive models that may improve the understanding and practical implementation of this technology.

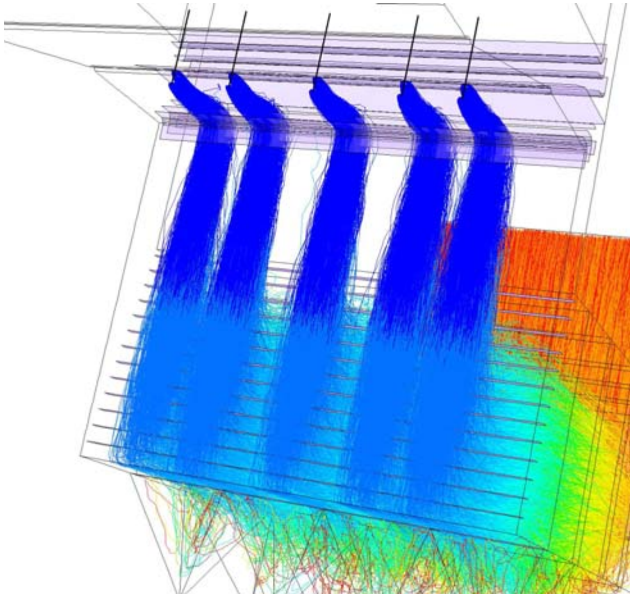
This presentation describes the development of an advanced model of in-flight mercury capture based on Computational Fluid Dynamics (CFD). The model makes detailed predictions of the in-duct spatial distribution and residence time of sorbent, as well as predictions of mercury capture efficiency for particular sorbent flow rates and injection grid configurations. Hence, CFD enables cost efficient optimization of sorbent injection systems for mercury control to a degree that would otherwise be impractical both for new and existing plants. In this way, modeling tools may directly address the main cost component of operating an ACI system – the sorbent expense. A typical 300 MW system is expected to require between $1 and $2 million of sorbent per year, and so even modest reductions (say 10-20%) in necessary sorbent feed injection rates will quickly make any optimization effort very worthwhile.

There are few existing models of mercury capture, and these typically make gross assumptions of plug gas flow, zero velocity slip between particle and gas phase, and uniform sorbent dispersion. All of these assumptions are overcome with the current model, which is based on first principles and includes mass transfer processes occurring at multiple scales, ranging from the large-scale transport in the duct to transport within the porous structure of a sorbent particle. In principle any single one of these processes could limit the overall capture of mercury. For example, capture may be severely limited in situations where the dispersion of sorbent is poor, or where adsorption rates are low because of relatively high temperatures.

Application examples taken from the DOE/NETL field test program were considered. The sites considered include Brayton Point, Meramec, Monroe, and Yates. Some general lessons learned concerning the impact of turbulence and flow stratification on dispersion and capture will be presented.

CFD Modeling for Mercury Control Technology





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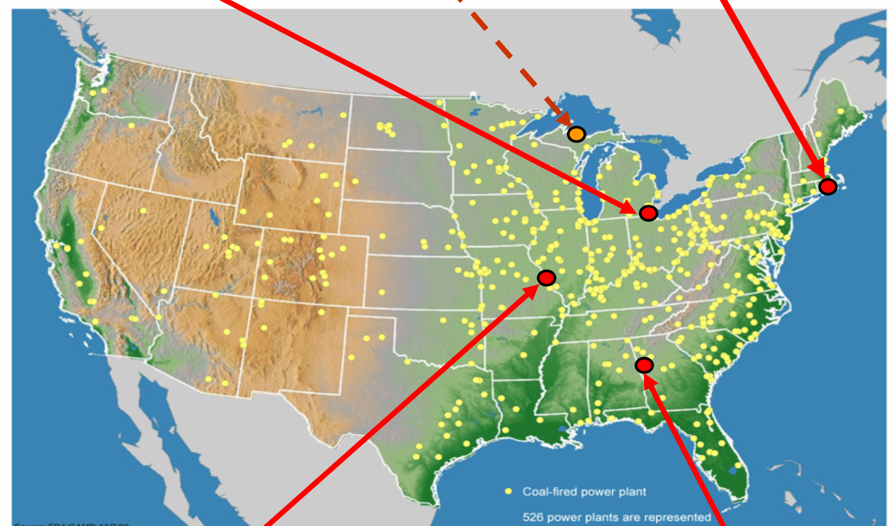
Background and Motivation

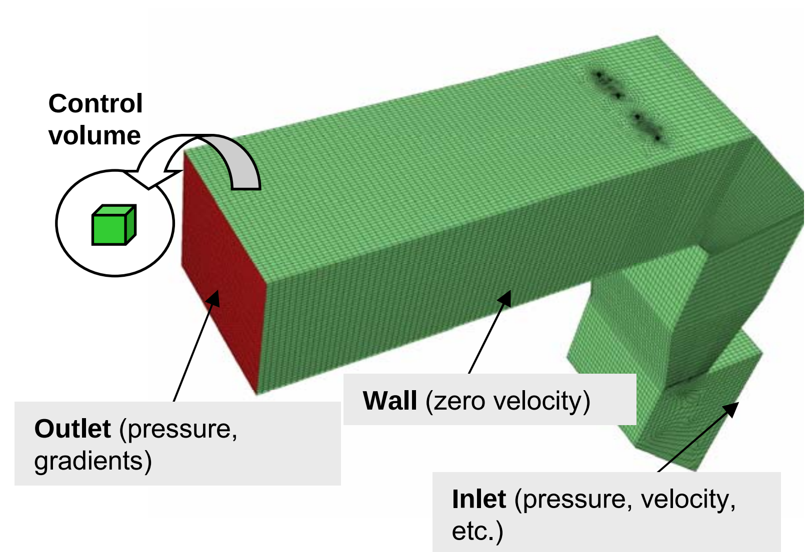
- There are 1,100+ coal-fired units in the United States
- These account for ~40% of man-made mercury emissions
- A typical 300 MW power plant will require between $1 and $2 million of sorbent per year
- CFD enables optimization of capture processes and may substantially reduce the cost of CAMR compliance
- Have provided flow modeling support for DOE/NETL field test sites over the past three years



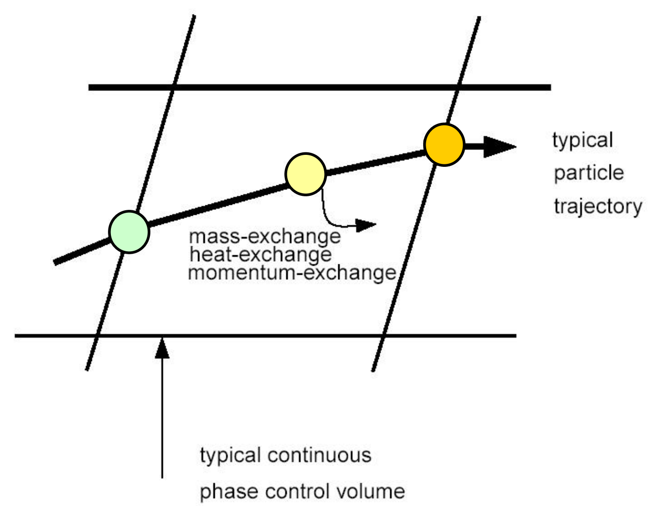
U.S. Coal-Fired Power Plants

Modeling Mercury Transport and Capture

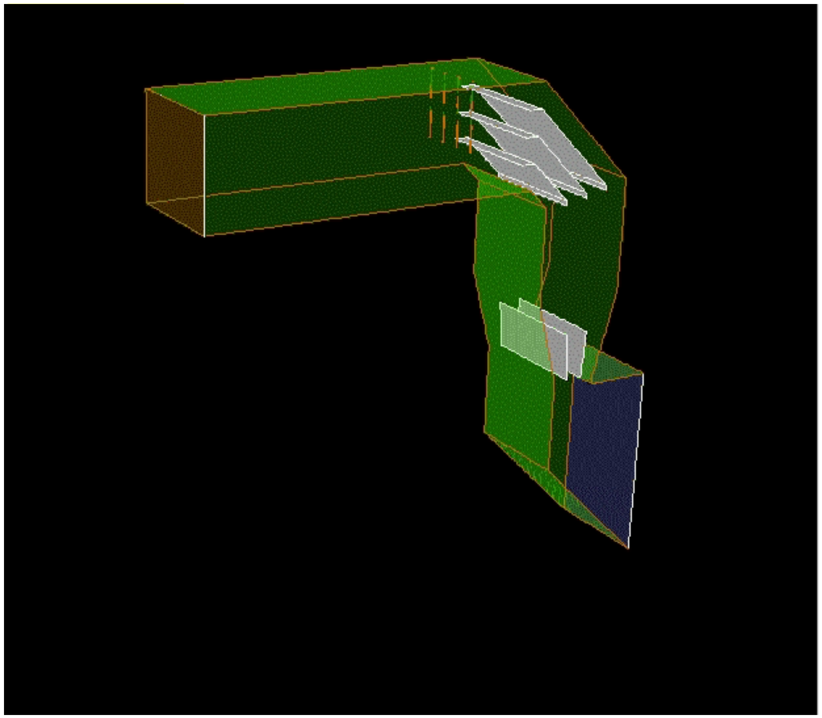
- **Distinct mass transfer processes**
  - These occur on multiple scales
  - Any single process could limit the overall capture of mercury



1. Injection and dispersion of solids
2. Duct-scale transport of gaseous mercury species (convection/diffusion)
3. Mass transfer from gas phase to external sorbent surface (film transport)
4. Pore diffusion through sorbent's interior
5. Surface adsorption on internal sites



Modeling Mercury Transport and Capture (2)

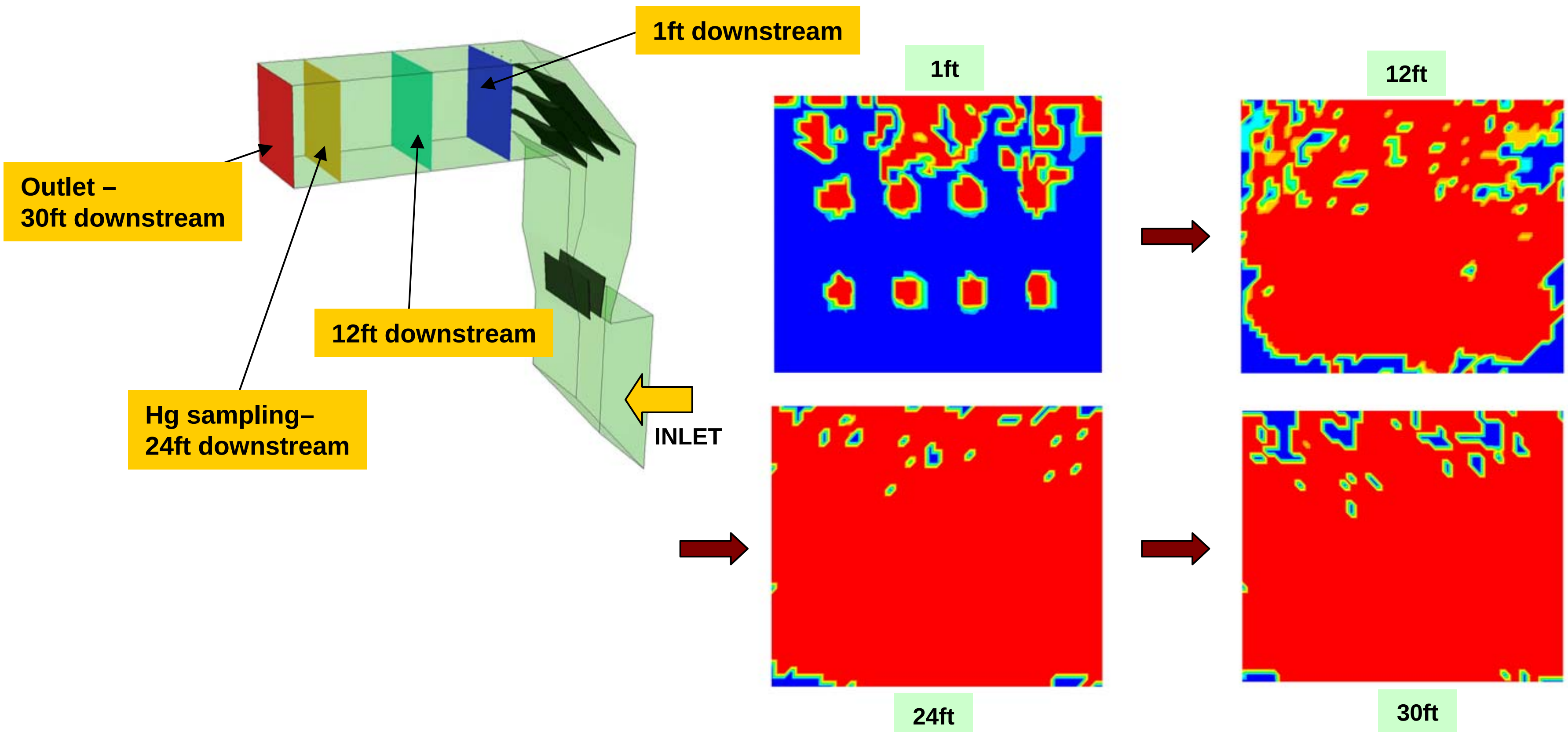


Brayton Point

Trajectories of injected sorbent, colored by residence time

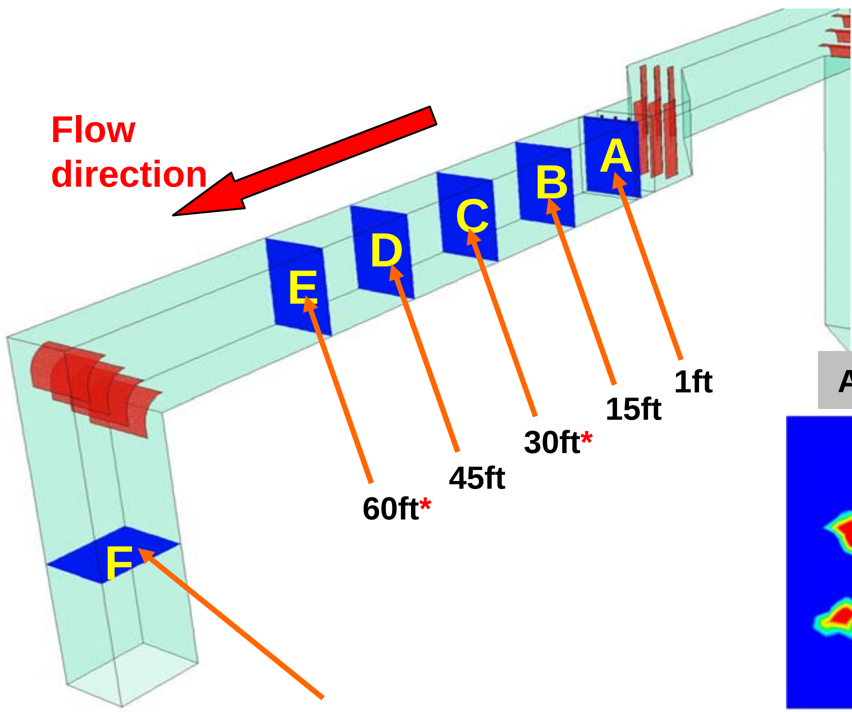
- **Gas phase conditions**
  - Velocity
  - Temperature
  - Mercury concentrations [$\mu g/m^3$] (Elemental/oxidized species)
  - (Pressure, turbulence params.)
- **Solid phase (sorbent) conditions**
  - Dispersion
  - Residence time
  - Where the capture takes place
- **CFD allows fast what-if studies**
  - Optimize injection systems
  - Significant savings over “build and test”

Brayton Point Dispersion Patterns

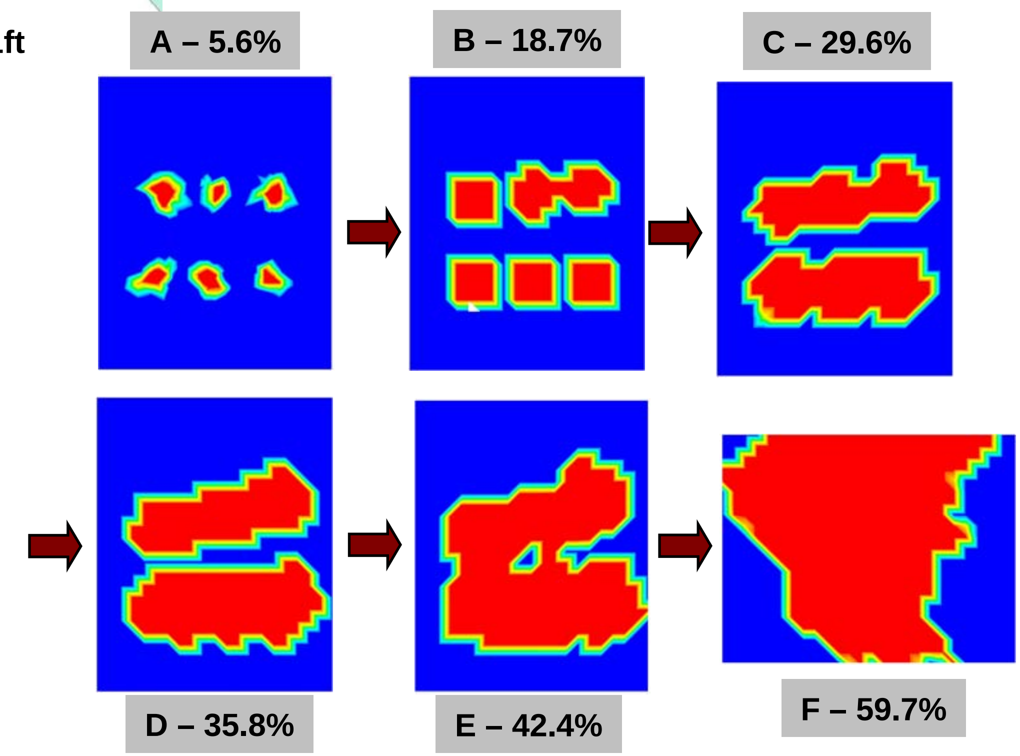


Coverage with >10% of average sorbent conc.

Meramec Dispersion Patterns



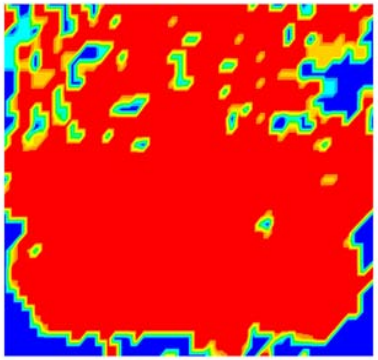
Coverage with >10% of average sorbent conc.



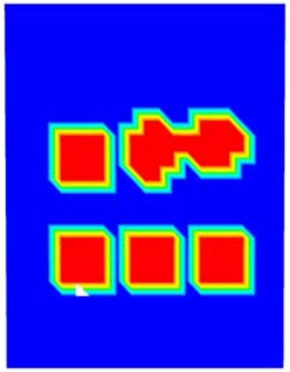
Sorbent Coverage at Brayton Point vs. Meramec

BRAYTON PT.

TKE ≈ 30.0 m^2/s^2



12ft after injection



15ft after injection

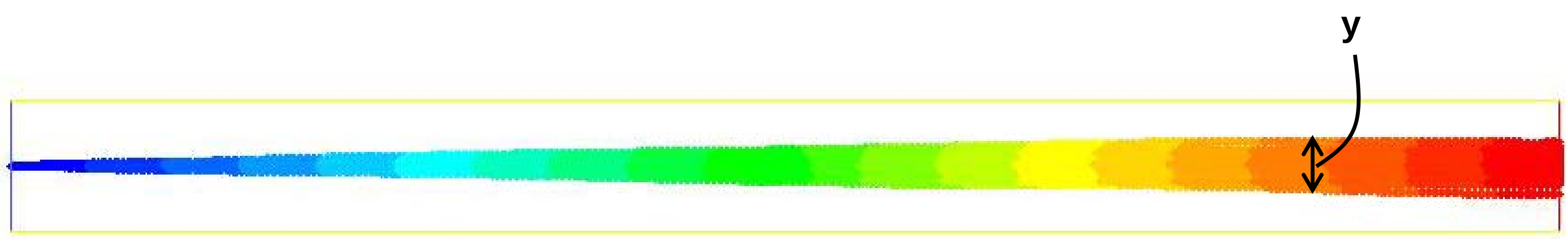
MERAMEC

TKE ≈ 1.0 m^2/s^2

Downstream Distance from Injection	*Brayton Point* Coverage Fraction		*Meramec* Coverage Fraction		Downstream Distance from Injection
	>100% avg.	>10% avg.	>100% avg.	>10% avg.	
1ft	0.069	0.221	0.049	0.056	1ft
12ft	0.224	0.840	0.125	0.187	15ft
30ft	0.307	0.944	0.164	0.296	30ft

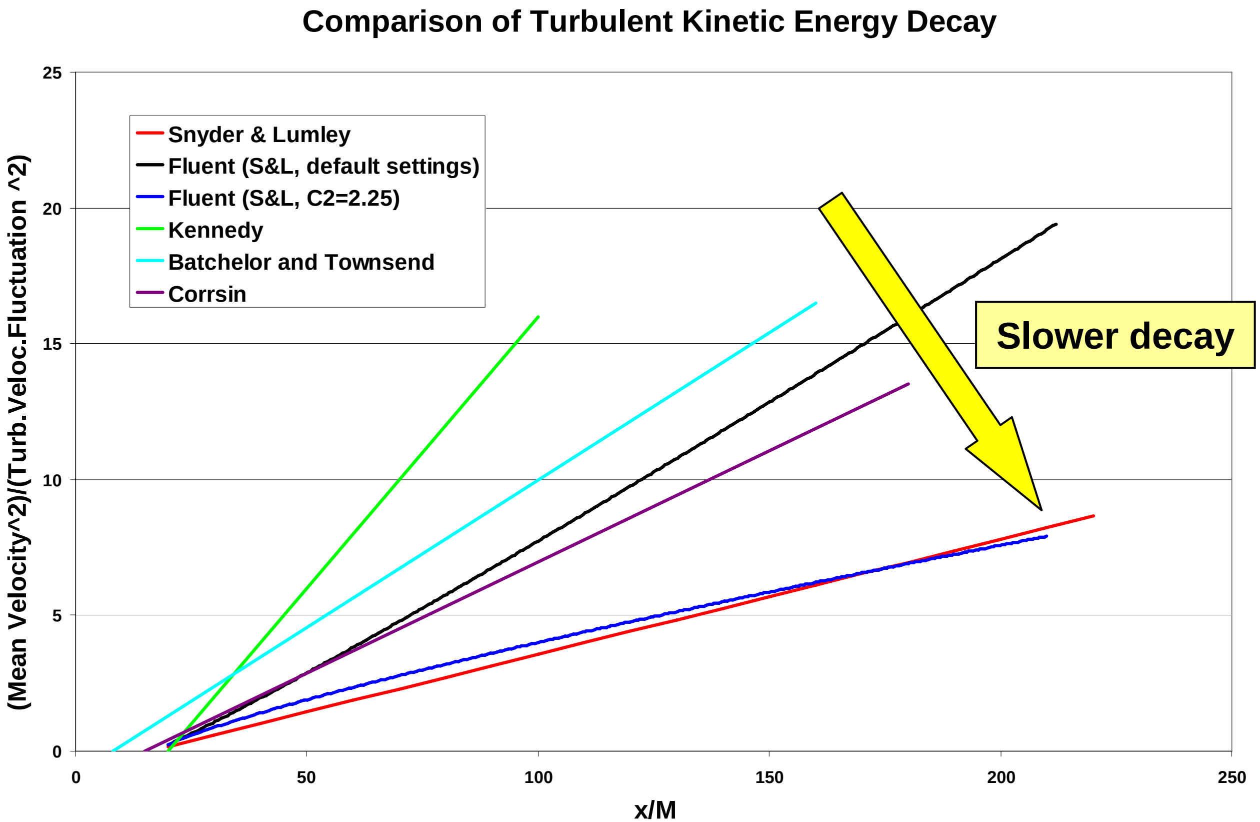
Validation of Discrete Particle Model

- **Can these predictions of sorbent dispersion be trusted?**
  - Dispersion data not available for real power plants
  - Circumstantial evidence exist in the form of dispersion results that match capture stratification patterns at Monroe field test site
  - A more thorough model validation required
- **Model validation based on well-documented experiments ***
  - Dispersion of particle jet in isotropic turbulence
  - Turbulence is generated in experiment using a screen
  - Turbulence intensity and decay hereof also measured



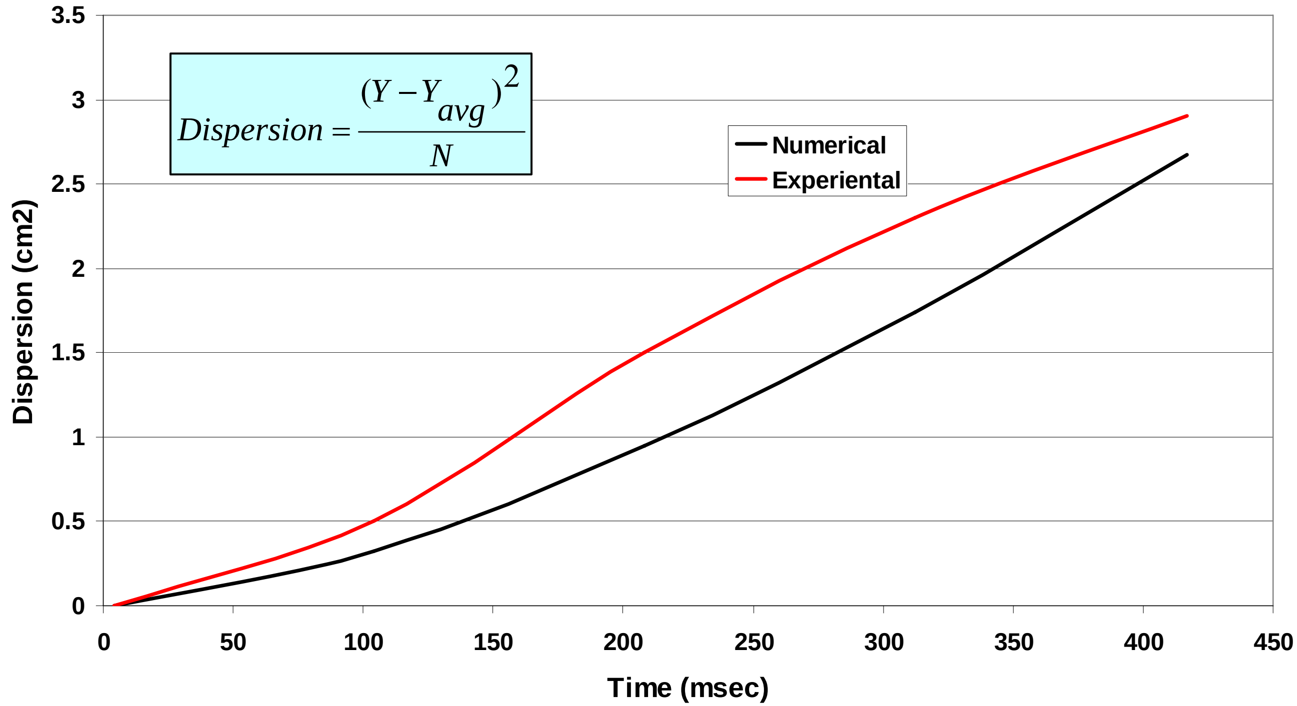
* **W.H. Snyder and J.L. Lumley :** "Some measurements of particle velocity autocorrelation functions in a turbulent flow", Journal of Fluid Mechanics, 1971, vol. 48 (No.1), pp 41-71.

Validation of Discrete Particle Model (2)



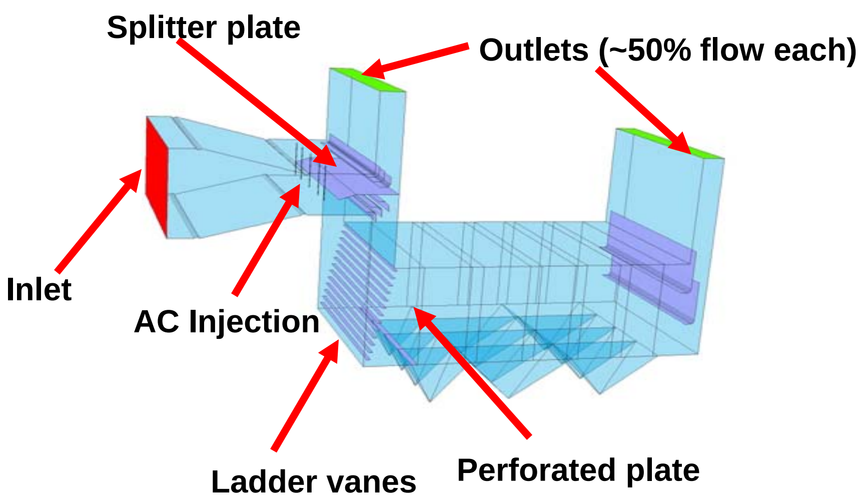
- **Decay of turbulence is relatively slow in Snyder & Lumley experiments**
  - Fluent with standard kε–model compares well with experiments
  - Turbulent decay matched by decreasing dissipation of turbulence in kε–model

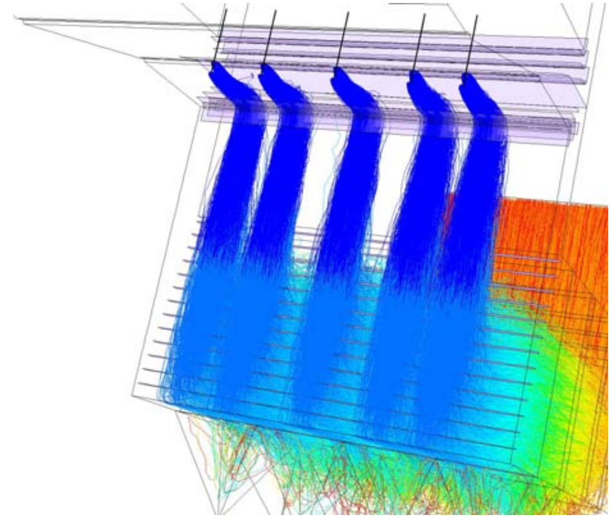
Validation of Discrete Particle Model (3)

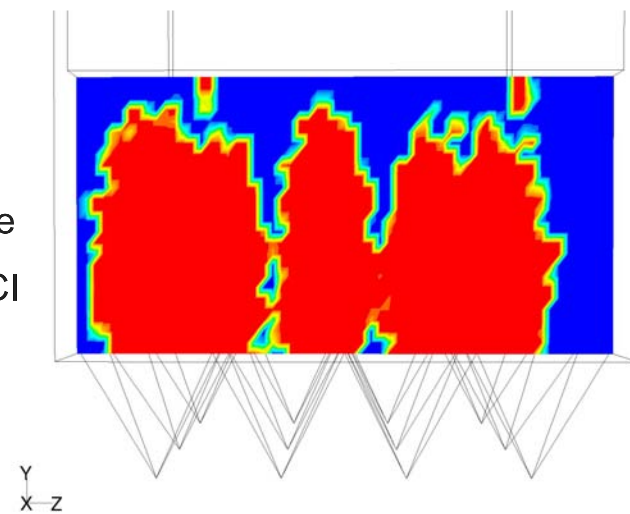


- **In this case CFD under-predicts the particle dispersion (by 5 … 30%)**
- **Second validation case involving sheared jets under investiagation**
  - This case should closer mimic flow conditions in a utility duct

DTE Energy’s Monroe Plant – ACI testing



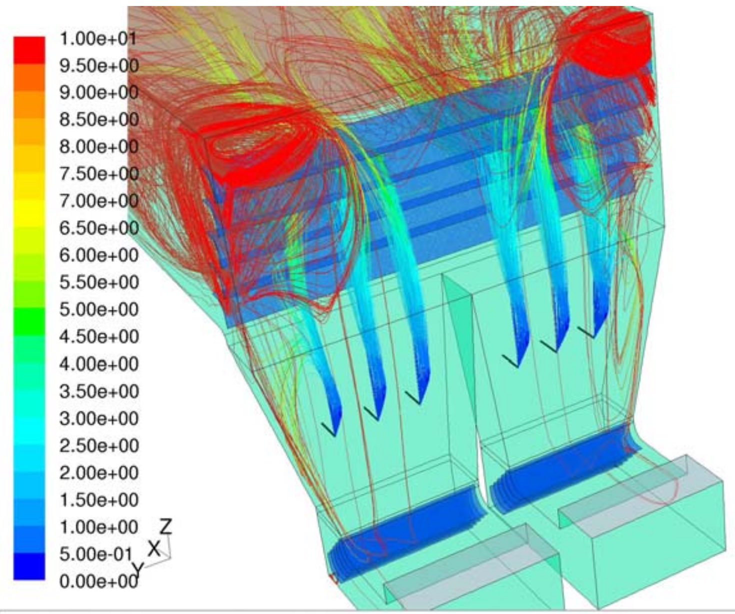




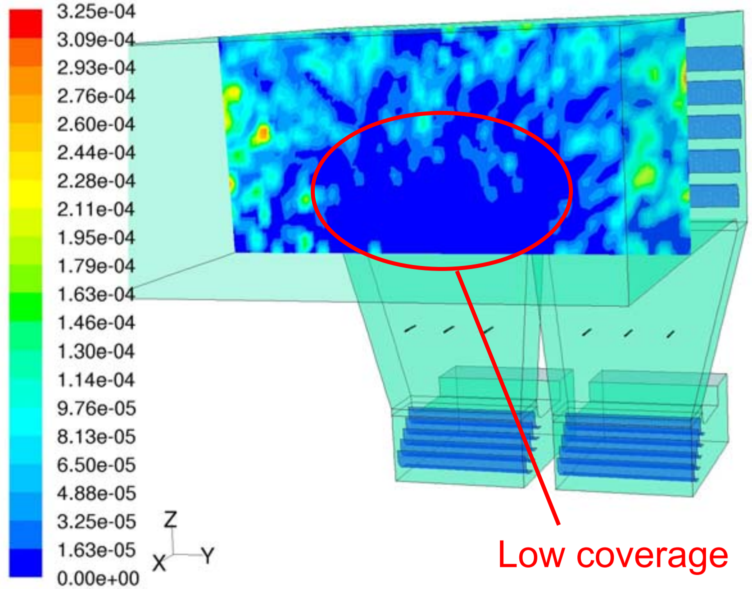
- Monroe plant has a very wide rectangular duct (51.5ft)
- Major stratification problems (temperature/sorbent/capture)
- Five multi-nozzle injection lances provide only partial coverage
- Stratification causes packages of gas to pass untreated by ACI
- Overall CFD predictions agree with outlet mercury sampling and analysis of hopper ash mercury content

Southern Co.'s Yates (Unit 1) – ACI Field Test Support

- **Maximum capture rates achieved during field tests: 55…60%**
  - Removal plateaus at high feed rates
  - Similar results with three different sorbents (Darco-Hg, HOK, NH Carbon)
  - Could this be a question of poor sorbent dispersion?



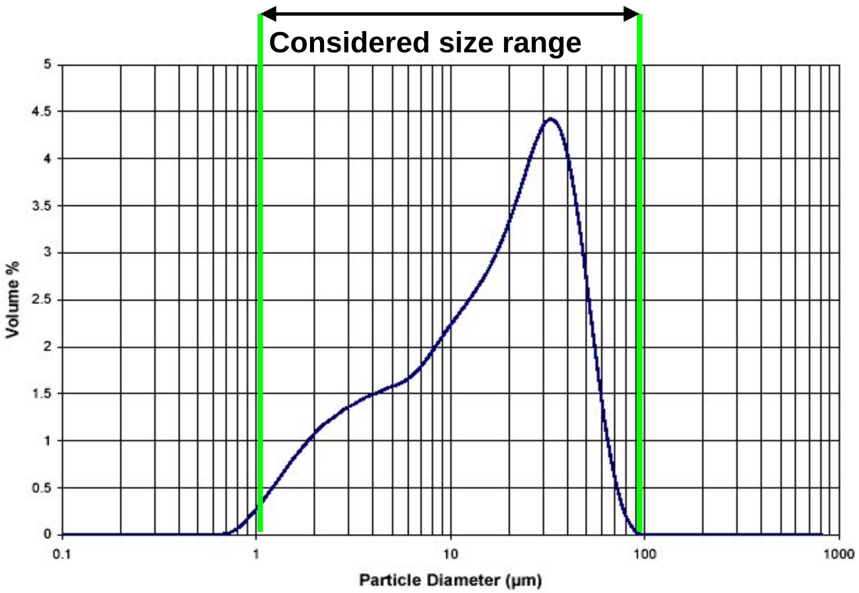
Particle Traces Colored by Particle Residence Time May 16, 2006
FLUENT 6.2 (3d, dp, segregated, ske)



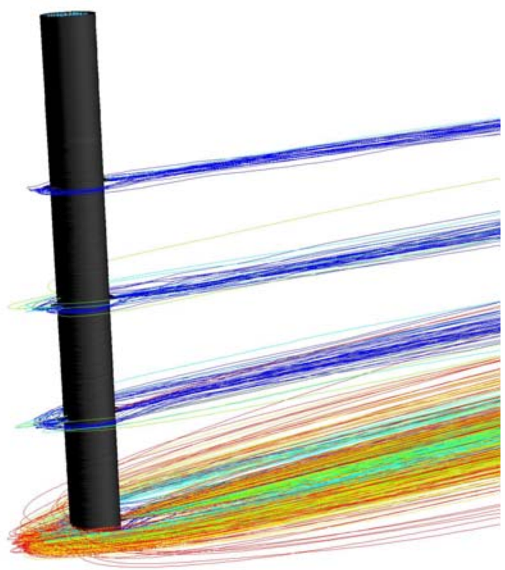
Contours of DPM Concentration (kg/m3) May 16, 2006
FLUENT 6.2 (3d, dp, segregated, ske)

Injection Lance Design

- **Determine sorbent split for multi-nozzle injection lances**
  - Flow modeling of lance interior



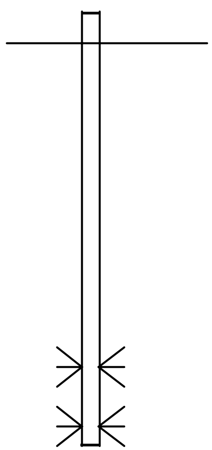
PSD for DARCO-Hg



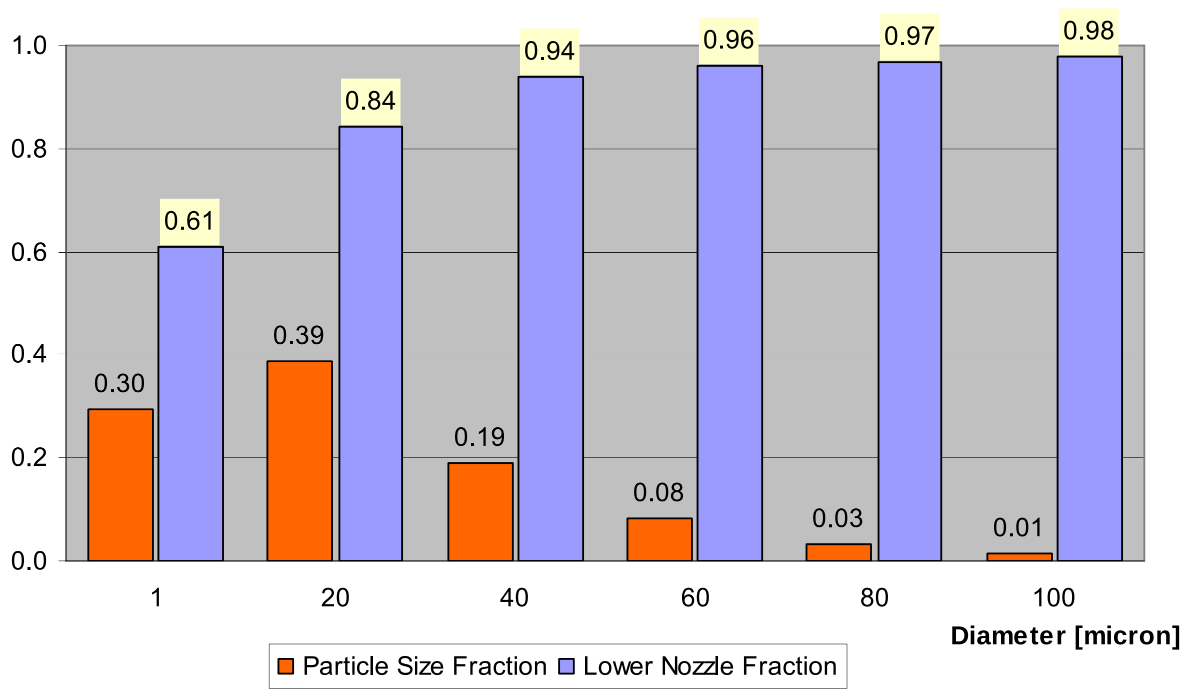
- **Ten size bins (d_p= 1 …100μm)**
- **Trajectory flow rates weighted by size distribution**

Injection Lance Design (2)

- **Multi-nozzle lances offer a false sense of security**
  - Sorbent split can be very uneven (here 81% exits lower set of nozzles)
  - Performance very similar to that of a much simpler single-nozzle lance
  - Staggered lance arrangements is a preferable approach to achieving good coverage from top-to-bottom of duct



Four-nozzle lance Used at DE-Monroe



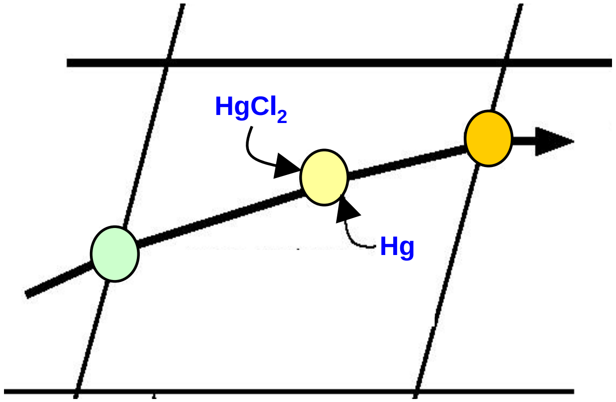
Capture Modeling – Simplifications and Inputs

- **Few existing models of mercury capture**
  - Typical simplifications include:
    - plug gas flow (1D models)
    - uniform sorbent dispersion
    - No velocity slip between particles and flue gas

1. Injection and dispersion of solids
2. Duct-scale transport of gaseous mercury species (convection/diffusion)
3. Mass transfer from gas phase to external sorbent surface (film transport)
4. Pore diffusion through sorbent's interior
5. Surface adsorption on internal sites

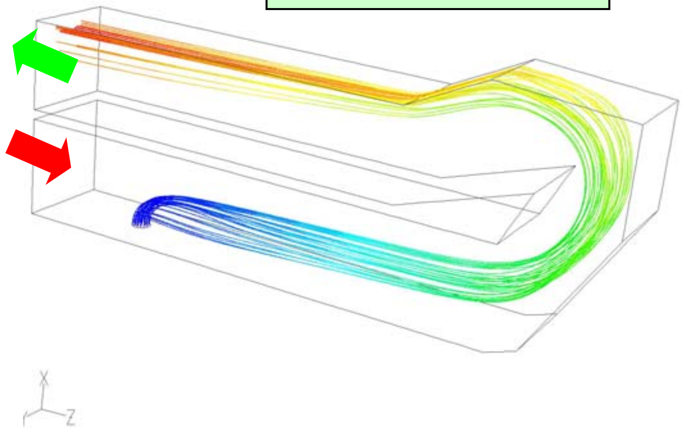
- **CFD-based model without these simplifications**
  - Based on first principles (conservation laws)
  - Considers adsorption of Hg(o) and $HgCl_2$

- **Mercury capture model inputs**
  - Duct geometry including injection gear
  - Flue gas mass flow rates
  - Inlet temperatures (constant or profiles)
  - Sorbent particle size distribution
  - Sorbent feed rates
  - Mercury inlet concentration [$\mu g/m^3$]
  - Oxidation fraction

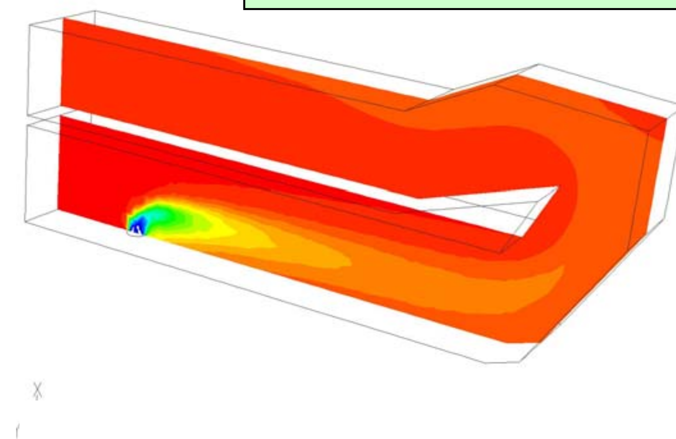


Capture Modeling – Example

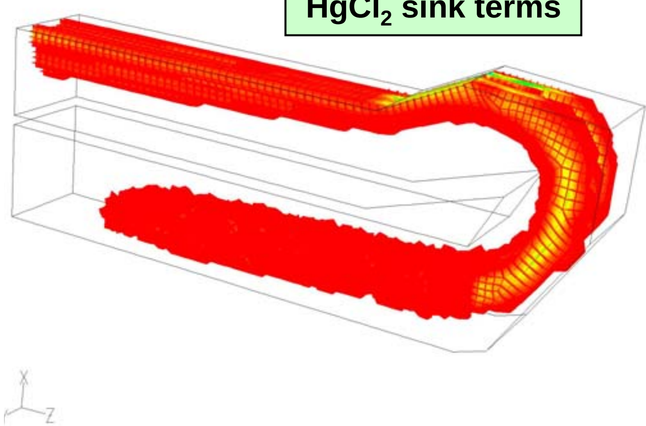
Sorbent trajectories



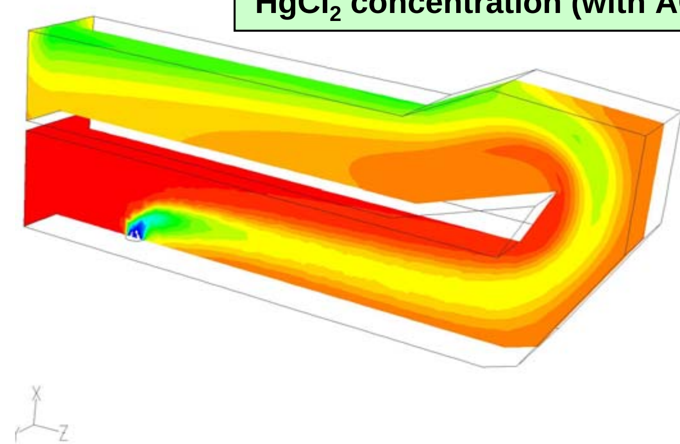
$HgCl_2$ concentration (no ACI)



$HgCl_2$ sink terms



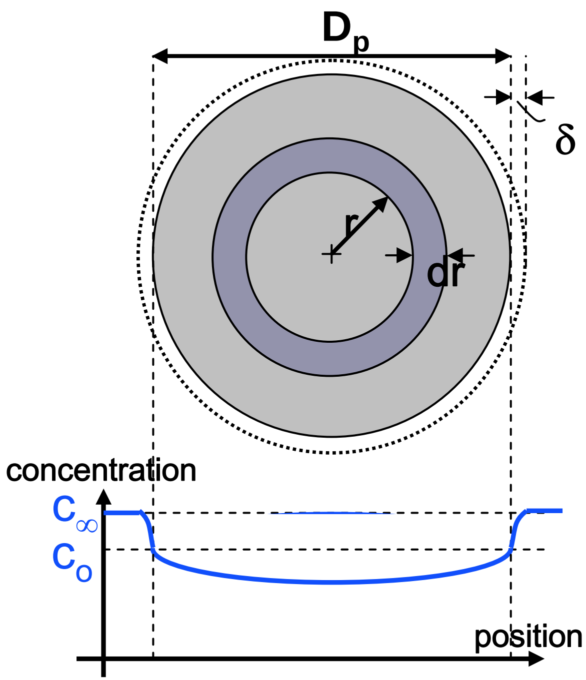
$HgCl_2$ concentration (with ACI)

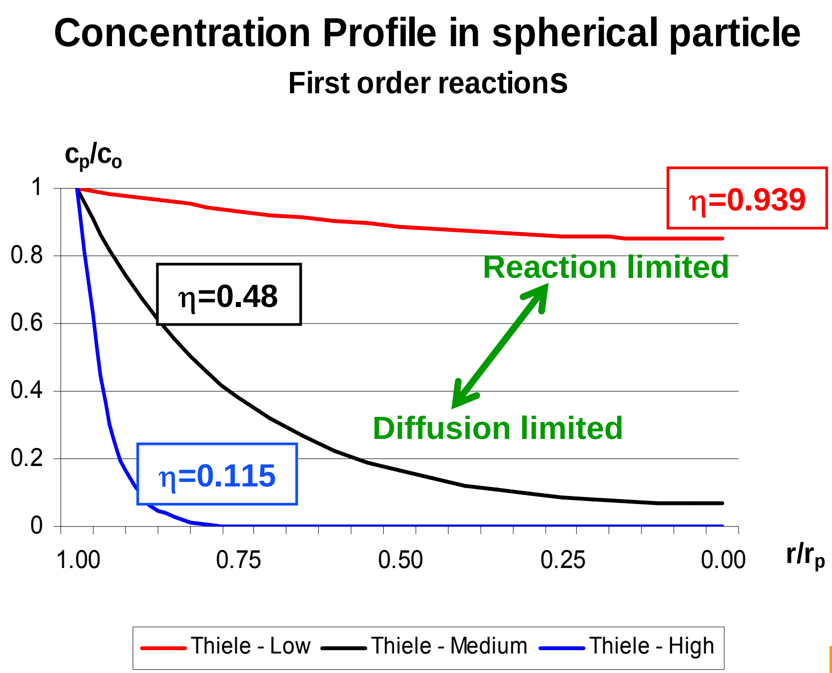


Capture Modeling – Sorbent Interior

- **Mercury species transport by porous diffusion**
  - Less diffusive mode limiting (Molecular or Knudsen Diffusion)

$$\frac{\epsilon_p}{\tau_p}\left(\frac{1}{D_g}+\frac{1}{D_{Kn}}\right)^{-1}$$





Thiele Modulus:

$$\Phi = r_p\sqrt{\frac{k_{ad}}{D_{eff}}}$$

Capture Modeling – Surface Adsorption

- **Mercury adsorption rates computed using Langmuir isotherms**
  - Separate isotherm expression for each mercury species
  - Capture by UBC may be accounted for by separate particle stream with own isotherm

- **Langmuir: net adsorption rate = forward rate (k_1) minus desorption rate (k_2)**

$$\Re = k_1 \omega_{max} [1 - \theta] c_{Hg} - k_2 \omega_{max} \theta$$

  - Here θ is the sorbent utilization (ω / ω_{max}), ie. fraction of occupied sites
  - ω_{max} is the maximum number of available sites (sorbent capacity)

- **Isotherm parameters (ω_{max}, k_1, and $b = k_1/k_2$) are temperature-dependent**
  - Getting proper isotherm data for a sorbent is challenging
  - When determined from packed bed breakthrough curves, adsorption process is essentially lumped with film transfer and pore diffusion

Conclusions and Future Work

- **CFD enables cost-effective optimization of injection grids for ACI**
  - Directly addresses the major cost component of this technology (sorbent cost)
- **Capture model shortcomings to overcome**
  - Lack of accurate adsorption rates hurts predictions of capture efficiency
  - Effects of flue gas chemistry (eg. Cl and SO_3) not accounted for
    - Mercury Speciation is frozen (prescribed at inlet)
    - Heterogeneous reaction kinetics appears to be crucial
    - Other adsorbates competing for activated sites
  - Identify strongly reduced reaction mechanism for mercury speciation and adsorption
    - NETL partnership with Clean Coal Center at University of Utah
- **Continued Field Test Modeling Support**
  - Currently building model for We Energies' Presque Isle TOXECON
  - Phase III DOE/NETL field test site(s)